

Supporting Information for Publication:

Photophysical and Theoretical Insights on Fullerene/Zincphthalocyanine Supramolecular Interaction in Solution

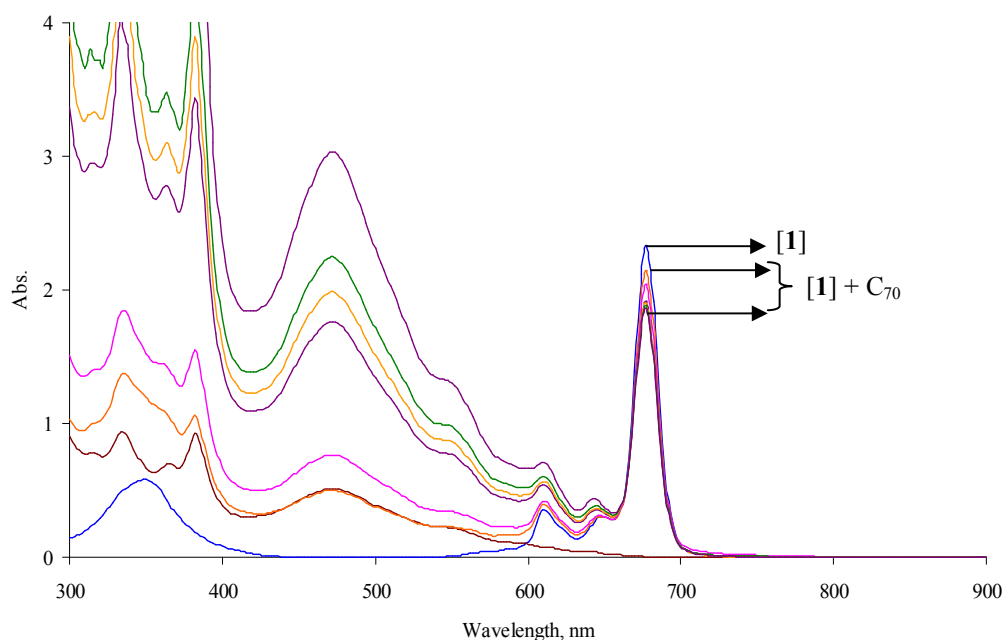
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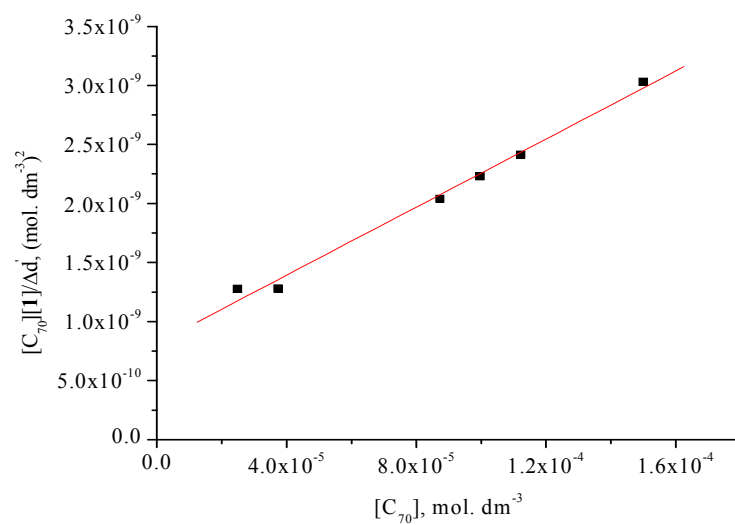
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Table 1S. HOMO & LUMO energy done by HF calculations for uncomplexed **1**, uncomplexed C₆₀, uncomplexed C₇₀, C₆₀/**1** and C₇₀/**1** systems done in *vacuo*.

System	HOMO & LUMO energy (in eV) done by HF calculations in <i>vacuo</i>
1	$E_{\text{HOMO}} = -5.2903$ $E_{\text{LUMO}} = -0.0175$
C ₆₀ - 1	$E_{\text{HOMO}} = -5.3013$
	$E_{\text{LUMO}} = -0.6592$
C ₇₀ - 1	$E_{\text{HOMO}} = -5.3039$
	$E_{\text{LUMO}} = -0.8506$
C ₆₀	$E_{\text{HOMO}} = -8.2755$ $E_{\text{LUMO}} = -0.7690$
C ₇₀	$E_{\text{HOMO}} = -7.9171$ $E_{\text{LUMO}} = -0.9531$

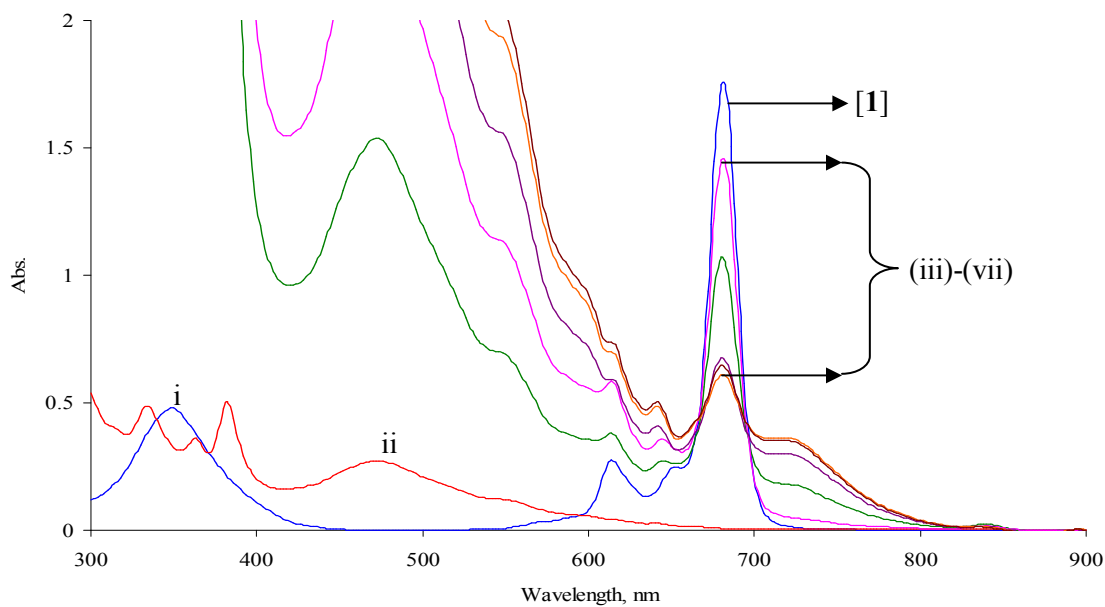


(a)

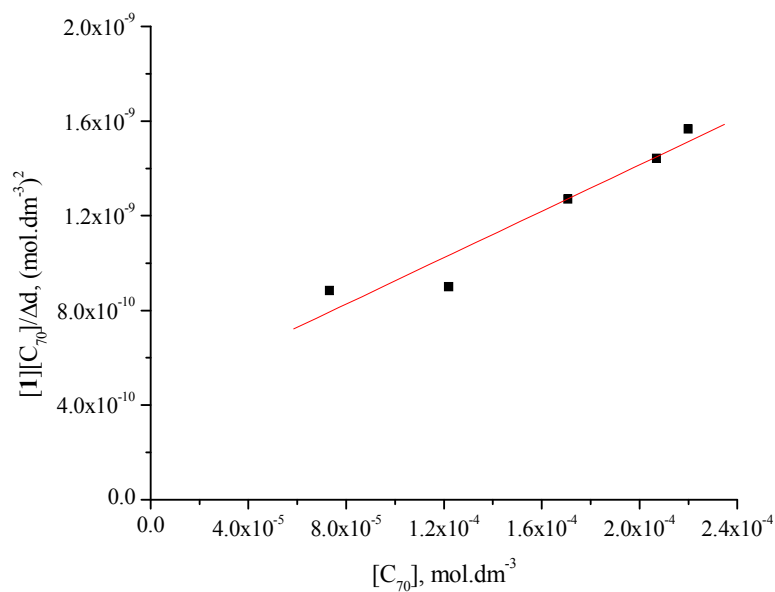


(b)

Fig.1S. (a) UV-Vis titration experiment of $C_{70}/\mathbf{1}$ complex recorded in toluene medium against solvent as reference by maintaining a constant concentration of $\mathbf{1}$ ($1.0 \times 10^{-5} \text{ mol}\cdot\text{dm}^{-3}$); the concentration of C_{70} increases (from bottom to top) in the range of 2.50×10^{-5} to $15.00 \times 10^{-5} \text{ mol}\cdot\text{dm}^{-3}$; (b) BH plot of $C_{70}/\mathbf{1}$ system recorded in toluene medium at 298K.



(a)



(b)

Fig. 2S. (a)UV-Vis titration curve of $C_{70}/\mathbf{1}$ system recorded in DCB; in Fig. 2S (i) uncomplexed $\mathbf{1}$ ($8.85 \times 10^{-6} \text{ mol}\cdot\text{dm}^{-3}$), (ii) uncomplexed C_{70} ($7.32 \times 10^{-5} \text{ mol}\cdot\text{dm}^{-3}$), and (iii)-(vii) mixture of C_{70} and $\mathbf{1}$ in which the concentration of C_{70} varies in the range of 7.32×10^{-5} to $2.20 \times 10^{-4} \text{ mol}\cdot\text{dm}^{-3}$; (b) BH plot of $C_{70}/\mathbf{1}$ system in DCB.

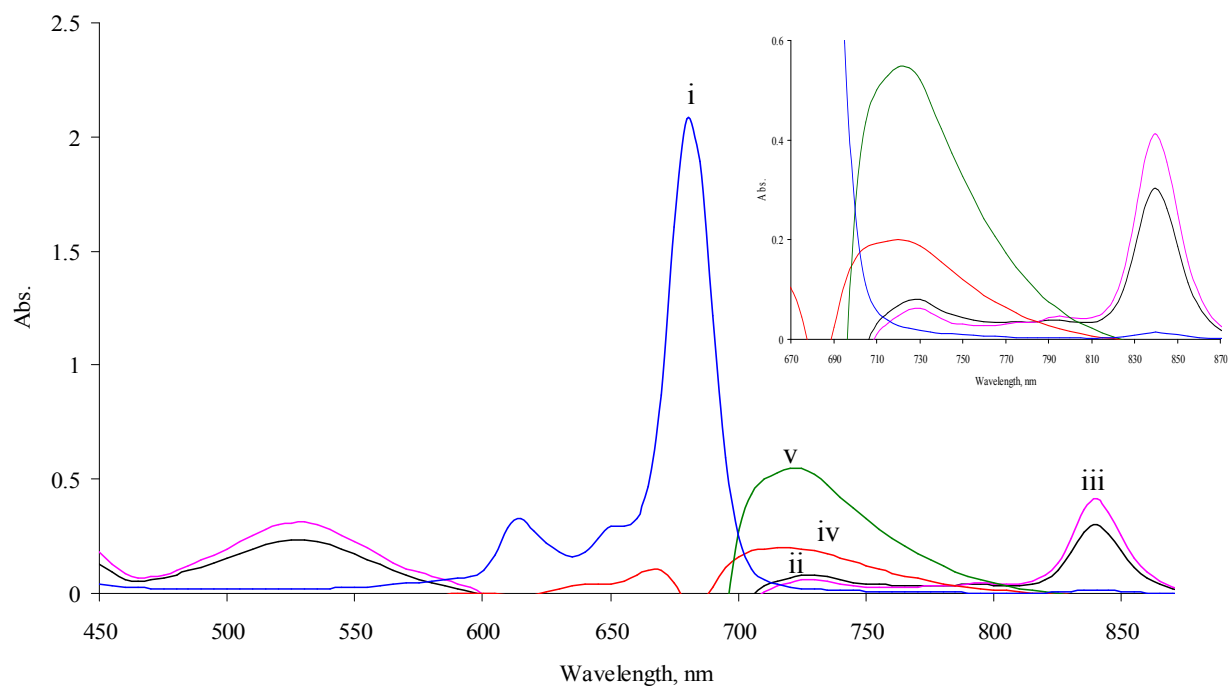


Fig. 3S. UV-vis absorption spectra of (i) **1** (1.30×10^{-5} mol. dm $^{-3}$), (ii) DDQ (1.17×10^{-4} mol. dm $^{-3}$) + **1** (1.30×10^{-5} mol. dm $^{-3}$), (iii) *o*-chloranil (7.85×10^{-4} mol. dm $^{-3}$) + **1** (1.30×10^{-5} mol. dm $^{-3}$), (iv) *p*-chloranil (9.50×10^{-4} mol. dm $^{-3}$) + **1** (1.30×10^{-5} mol. dm $^{-3}$) and (v) TCNQ (4.75×10^{-4} mol. dm $^{-3}$) + **1** (1.30×10^{-5} mol. dm $^{-3}$) in DCB medium.

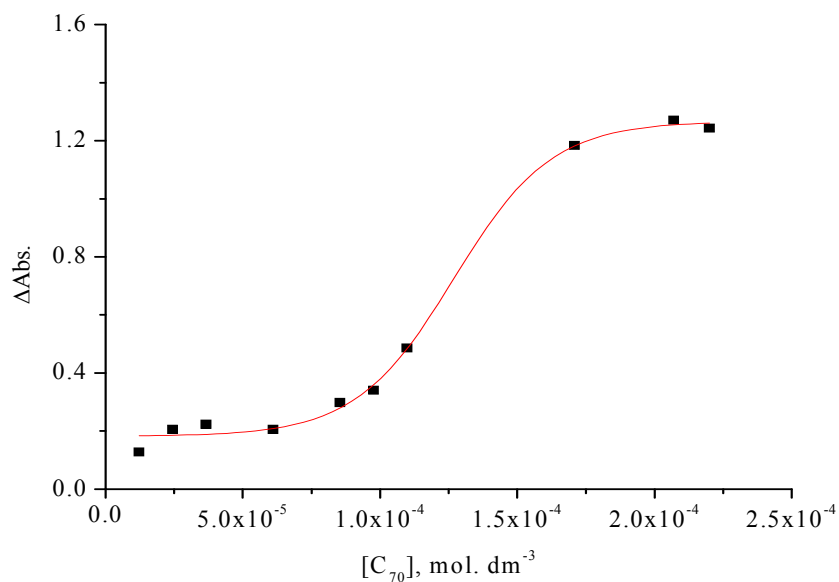
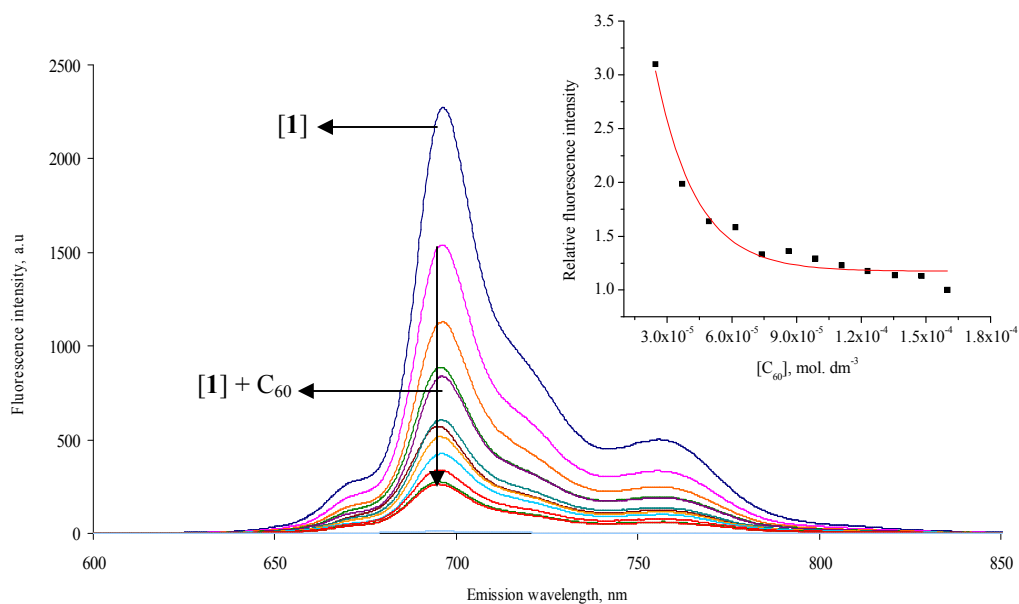
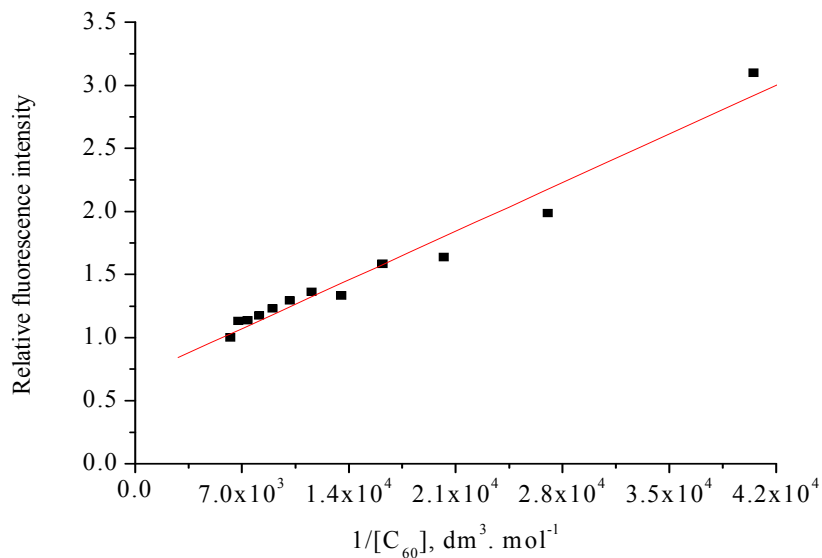


Fig. 4S. Saturation of absorption for C₇₀/**1** system in DCB

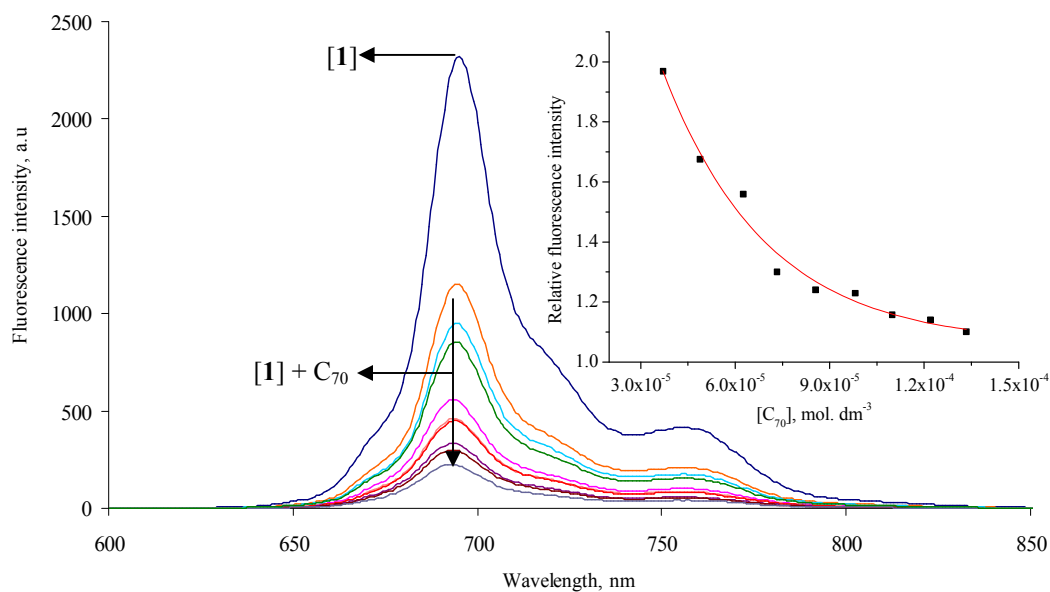


(a)

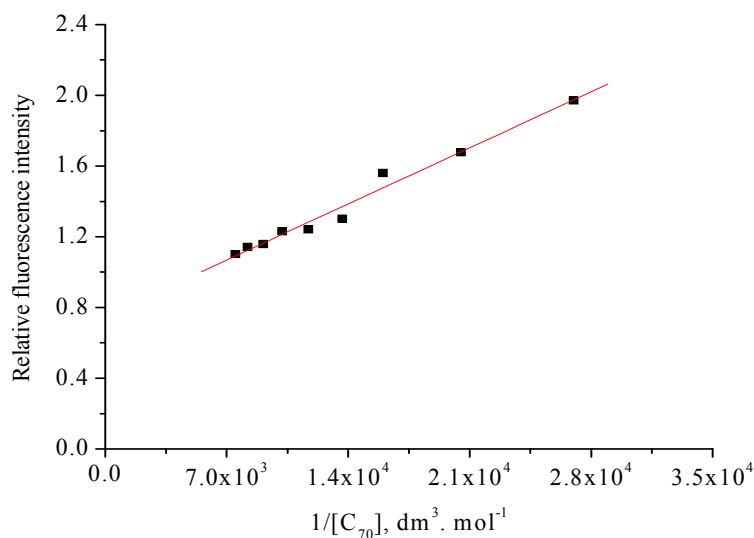


(b)

Fig. 5S. (a) Steady state fluorescence spectral variation of **1** ($1.0 \times 10^{-5} \text{ mol} \cdot \text{dm}^{-3}$) in presence of C_{60} in DCB medium, the concentrations of C_{60} from top to bottom are as follows: 2.47×10^{-5} , 3.7×10^{-5} , 4.95×10^{-5} , 6.17×10^{-5} , 7.40×10^{-5} , 8.64×10^{-5} , 9.87×10^{-5} , 1.10×10^{-4} , 1.23×10^{-4} , 1.35×10^{-4} , 1.48×10^{-4} and $1.60 \times 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$; plot of Relative Fluorescence Intensity vs. $[\text{C}_{60}]$ for $\text{C}_{60}/\mathbf{1}$ system in DCB medium is shown in inset; and (b) BH fluorescence plot of $\text{C}_{60}/\mathbf{1}$ system in DCB medium.



(a)



(b)

Fig. 6S. (a) Steady state fluorescence spectral variation of **1** ($8.85 \times 10^{-6} \text{ mol}\cdot\text{dm}^{-3}$) in presence of C_{70} in DCB medium; the concentrations of C_{70} from top to bottom are as follows: 3.70×10^{-5} , 4.88×10^{-5} , 6.25×10^{-5} , 7.32×10^{-5} , 8.55×10^{-5} , 9.80×10^{-5} , 1.09×10^{-4} , 1.22×10^{-4} , 1.33×10^{-4} and $1.46 \times 10^{-4} \text{ mol}\cdot\text{dm}^{-3}$; plot of Relative Fluorescence Intensity vs. $[\text{C}_{70}]$ for $\text{C}_{70}/\mathbf{1}$ system in DCB medium is shown in inset; and (b) BH fluorescence plot of $\text{C}_{70}/\mathbf{1}$ system in DCB medium.